

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

## Model Results

**Predicted value:** 277 °C

**Global applicability domain:** Outside

**Local applicability domain index:** 1.59e-01

**Confidence level:** 7.63e-01

## Nearest Neighbors from the Training Set

Image not found

Diphenylurea

**Measured:** 262

**Predicted:** 269

Image not found

Benzoic acid, 2-phenylhydrazide

**Measured:** 314

**Predicted:** 306

Image not found

N-(4-Bromophenyl)urea

**Measured:** 260

**Predicted:** 256

Image not found

1-Phenylurea

**Measured:** 238

**Predicted:** 247

Image not found

2-Nitrobenzamide

**Measured:** 317

**Predicted:** 310